

REMARKS

Claims 1-100 are pending and are rejected. Claims 1, 3, 6, 21, 23-36, 39-42, 53-66, 90-91, 94, 96 and 98 have been amended. Claims 2, 69-89, 95, 97 and 99-100 have been cancelled without prejudice in order to facilitate prosecution. No new matter has been added. The applicant respectfully requests reconsideration and allowance of all claims in light of the amendments and of the following remarks.

1. Telephonic Interview

The applicant thanks the Examiner for extending the courtesy of a telephonic interview on September 10, 2003. During the interview, the applicant's representative explained the scientist's interaction with the computer program product recited in claim 1 – specifically, the scientist's role in defining the set of experimental parameters, sampling patterns and constraints recited in claim 1, as discussed in more detail below. The applicant's representative proposed amending claim 1 to expressly recite that these features of the claim were defined based on user input, as reflected in the current amendment to claim 1, and pointed to various parts of the specification believed to support the enablement of the claim as amended. No agreement was reached.

2. Claim Objections

Claims 56 and 57 were objected to as lacking a period following the number of the respective claim. Claims 56 and 57 have been amended to add the period in question. The applicant therefore requests that the objections be withdrawn.

3. Rejections under Section 112

a. Rejections under Section 112, First Paragraph

Claims 1-100 are rejected under the first paragraph of 35 U.S.C. § 112 as allegedly containing subject matter that is not described in the specification in such a way as to enable one skilled in the art to make and use the invention. The applicant respectfully disagrees.

As explained in the applicant's specification, the efficient exploration of high-dimensional parameter spaces using combinatorial and high-throughput techniques depends on the ability to choose experimental points in the parameter space for maximum information content. *See* Specification at page 11, lines 25-26. As the specification also explains, this amounts to the treatment of the parameter space as a volume, and the choice of experiments to efficiently populate this volume. *Id.* at lines 27-29. By contrast, traditional experimental science has been done using experiments designed so that a desired property is measured as a function of a particular parameter, typically with all other parameters being held constant. *See id.* at page 10, lines 20-22. Since virtually any property is influenced by more than a single parameter, these techniques result in the observation of a two-dimensional slice through the parameter space defined by all of the parameters that can play a role in defining the property in question. *Id.* at page 10, lines 23-28. Attempting to extrapolate multidimensional relationships from these two-dimensional slices can result in the omission of significant information. *Id.* at page 11, lines 10-16.

The invention recited in claim 1 is an experiment design tool that can be used by the scientist to help in the process of efficiently populating the experimental parameter space, and to avoid the two-dimensional limitations of traditional experimental approaches. To that end, claim 1 recites a computer program product for designing a set of experiments that is represented as a set of points in a multidimensional hyperspace defined by a set of experimental parameters. As amended, the claim is directed to a program that includes instructions operable to cause a programmable processor to receive input defining a set of experimental parameters, one or more sampling patterns, and one or more constraints. The processor generates an estimate of the practicability of a first (predecessor) set of experiments defined by the parameters, sampling patterns and constraints, and provides the estimate to a user. The processor receives input modifying the parameters, sampling patterns or constraints in response to the estimate, and generates an estimate of the practicability of a second (successor) set of experiments defined by the modified parameters, sampling patterns and constraints. In response to input approving of the second (successor) estimate (or a further successor estimate based on additional iterations),

the processor generates an experiment design including data representing a final set of experiments (*e.g.*, the experiments to be practiced).

Claim 1 is directed to a computer program product that can be used to design a set of experiments. The claim is enabled if one skilled in the art, having the benefit of the disclosure, would be able to make and use the invention without undue experimentation. In the software context, the Court of Appeals for the Federal Circuit has stated that “normally, writing code for such software is within the skill of the art, not requiring undue experimentation, once its functions have been disclosed.” *See Fonar Corp. v. General Electric Co.*, 107 F.3d 1543, 1549 (Fed. Cir. 1997) (addressing adequacy of disclosure of software under best mode requirement); *see also Northern Telecom, Inc. v. Datapoint Corp.*, 908 F.2d 931, 941 (Fed. Cir. 1990). Thus, the question here is whether the specification describes the functions to be performed by the claimed computer program product adequately to enable one skilled in the art to implement those functions in computer program code. The applicant submits that it does.

The Examiner states that undue experimentation would be required to practice the claimed invention in view of the alleged lack of direction or guidance presented in the specification, the absence of working examples, the alleged complex nature of the invention, the difficulties experienced in the prior art with respect to high dimensional experiment design, and the breadth of the claims. Specifically, the Examiner states that the claims “are not limited to well-understood chemical processes and encompass vast parameter spaces, irregular response surfaces, and large libraries” and concludes that the specification “does not provide exemplification or guidance on designing sets of experimental parameters for such situations.” Office Action, page 4. Although the claims are not limited to applications involving well-understood chemical processes – or to any particular type of chemistry, for that matter – the fact that the phenomena being investigated in a particular set of experiments may not be well-understood does not mean that implementing the claimed invention to define those experiments would be unduly difficult.

The claimed computer program product receives input defining the set of experimental parameters to be used in defining the set of experiments. Each parameter defines an axis of the parameter space in which the set of experiments will be defined. The specification explains that

these parameters can represent process parameters – for example, process conditions such as temperature, pressure, or annealing time – or physical parameters, such as the molecular weight, grain size, or identity of particular elements, compounds or compositions that will be used in the experiments. *See* page 28, lines 21-26. The choice of parameters in any given set of experiments depends on the nature of the experiments, and can require more or less insight into the underlying physics or chemistry, also depending on the particular experiments. The choice of parameters to define, however, is up to the scientist; all claim 1 requires is that the parameters be definable – that is, if the scientist can identify the parameters (and the sampling patterns and constraints), the claimed computer program product can use the parameters, in combination with sampling patterns and constraints, to define a set of experiments. Significantly, although underlying mechanisms for some chemical processes (*e.g.*, some chemical reactions) may not be well understood, the type of parameters that can influence such processes (*e.g.*, temperatures, pressures, reaction times, catalyst compositions, reactor designs, *etc.*) are typically well established for particular chemical processes of interest.

The input also defines one or more sampling patterns that define a sampling of each of the experimental parameters. These sampling patterns essentially determine how values for each parameter will be selected – that is, how the computer program product will select parameter values along each of the parameter axes to define points for inclusion in the set of experiments. The specification explains that the sampling patterns can be defined as fixed values, which can be absolute or relative, or as variable sampling patterns such as linear, logarithmic or higher order gradients, and describes an exemplary user interface for defining a simple gradient sampling pattern. *See* Specification at page 14, line 24-page 15, line 15; page 21, lines 7-20 & FIG. 6.

Finally, the input defines one or more experimental constraints that limit the set of experiments to a volume or volumes in the parameter space. These constraints define boundaries beyond which points that would otherwise be included in the set of experiments will instead be excluded. The specification identifies and describes the definition and function of a large number of different types of constraints, such as mixture constraints, composition constraints,

type constraints, and others. *See* Specification at page 16, line 16-page 19, line 4; page 21, line 21-page 23, line 5 & FIGS. 7-9.

The specification explains that, based on the defined parameters, sampling patterns and constraints, the design program generates an experiment design by performing a combinatorial expansion to identify a set of experiments (*e.g.*, involving different candidate materials). *See* Specification at page 19, lines 7-9. As one example of such an expansion, the specification explains that the program can do so “by counting through points in the parameter space corresponding to combinations of the specified parameter values and applying the specified constraints to each such point.” *Id.* at page 19, lines 9-11.

Moreover, the specification describes a particular embodiment of the invention in which the parameters, sampling patterns, and constraints are implemented as objects defined according to the object model illustrated in Figure 14. *See* Specification at page 28, line 9-page 32, line 5. As the specification explains, in this embodiment the parameters are represented by Parameter objects, sampling patterns are represented by Factor objects, and constraints are represented by Constraint objects. *Id.* at page 28, line 21-page 29, line 25. As the specification explains, Group objects associate Parameter objects with Factor objects, such that the Parameter objects identified in a particular Group will be present in the set of experiments according to the Factor object identified in that Group. *Id.* at page 29, lines 14-23. Factor objects define sampling patterns according to one or more Levels objects that identify the allowed levels for the corresponding parameter. *Id.* at page 29, lines 1-4. Constraint objects specify constraints for an identified list of Factor objects by defining a set of mathematical conditions that will be applied to values specified by the corresponding Factor levels. *Id.* at page 29, lines 24-27.

The specification gives a number of specific examples of how constraints can be implemented. Thus, for example, the specification explains that a constraint can be represented mathematically as a linear combination of factors and an upper limit and/or a lower limit on the values for those factors, such that the constraint evaluates to true if the value of the linear combination falls within the limits. *Id.* at page 29, lines 27-30. As another example, the constraint can be represented as a single set of levels for each Factor and can specify a distance criterion for each, such that the constraint evaluates to true based on where each Factor value

falls with respect to its distance from the specified levels. *Id.* at page 29, line 31-page 30, line 3. In still other examples, a constraint can specify a fixed ratio between Factors, such that it evaluates to true if the ratio is satisfied, and can specify non-numerical relationships as well. *Id.* at page 30, lines 3-6.

In this embodiment, a Composition object expresses how a set of parameters is combined to form an experiment design, with properties including a set of Groups (with associated Parameters and Factors), and one or more Constraint objects that define the constraints to be applied to the Groups. *See* Specification at page 30, lines 7-11. The specification explains that the Composition object has a Get_Basket function that returns the contribution of the particular Composition object to each experimental point in the expansion. *Id.* at page 31, lines 4-7. One implementation of the Get_Basket function is described in detail – specifically, that the function calculates a template design by building a set of nested loops over each Factor object level, evaluating each of the constraints listed in the Composition object for each combination of levels and adding to the experiment design an experimental point corresponding to the combination if all of the constraints evaluate to true. *Id.* at page 8-17. The template design is then used to generate a design for the parameter space points represented by the Composition object by replacing factors with corresponding parameters in the template design and replicating the template design for each set of parameters. *Id.* at page 31, line 29-page 32, line 3. A final experiment design can be generated by calling the Get_Basket function for each Composition object in a given Project. *Id.* at page 32, lines 3-5.

The applicant submits that this description, and particular the discussion of FIG. 14, would clearly demonstrate to one skilled in the art how to calculate a combinatorial expansion given definitions of a set of parameters, sampling patterns, and constraints, the result of which would be a set of experiments that populates the experimental parameter space as a volume, as opposed to a series of slices or projections.

The Examiner also suggests that one skilled in the art would not recognize how to determine claim 1's first estimate of practicability, "particularly where it is not merely a count of candidate materials that is acceptable or unacceptable to a user." The applicant notes that in fact every claim that recites determining an estimate of practicability expressly provides that the

estimate includes a count of the set of experiments defined by the parameters, sampling patterns and constraints. The applicant submits that, based, for example, on the discussion cited above, one skilled in the art would be able to determine such a count of the number of experiments required to implement an experiment design without undue experimentation. That the estimate might also include other information, such as a correlation between the time taken to calculate the combinatorial expansion and the expected time to actually perform the experiments represented by the experiment design, based, for example, on chemistry- and project-specific computational thresholds (*see, e.g.* Specification at page 19, lines 15-22) does not change this.

For at least these reasons, the applicant submits that the claims are enabled under section 112, paragraph 1, and requests that the enablement rejection be withdrawn.

b. Rejections under Section 112, Second Paragraph

Claims 1-100 are rejected under the second paragraph of 35 U.S.C. § 112 as allegedly being indefinite. The applicant respectfully disagrees.

The Examiner first points to the use of “designing a set of experiments” in each of the pending claims, and asks what information is to be generated to meet this limitation. The applicant first points out that the claims specify that the methods and computer programs of the present invention generate an experiment design that is “defined by the parameters, the sampling patterns, and the constraints”. Each of the independent claims has been amended to further recite that the experiment design includes data representing a final set of experiments, where the data includes “a plurality of sets of coordinates in the hyperspace defined by the set of experimental parameters, each of the sets of coordinates defining an experiment in the final set of experiments.” The applicant submits that this language makes it clear that the experiment design must include at least data defining sets of coordinates in the hyperspace defined by the experiment parameters, which sets of coordinates each represent an experiment in a final set of experiments of the experiment design. The Examiner suggests that the use of “including” in this context makes the claims indefinite, but the applicant submits that the claims clearly require data representing hyperspace coordinates as just described. That they may also include additional information does not render the claims indefinite.

The Examiner also seems to conclude that the use of “final set of experiments” renders the claims indefinite; the claims have been amended to clarify that the first and second estimates that are generated according to the present invention are estimates of the practicability of a first and second set of experiments, respectively, which can be “intermediate” sets of experiments as the Examiner suggests.

The Examiner states that the use of “one or more sampling patterns defining a sampling for each parameter” makes it unclear whether each parameter is associated with one particular sampling pattern or whether one parameter can have multiple sampling patterns at the same time. The language in question encompasses situations where a sampling pattern is defined for each parameter, but that it also covers cases where there are more or fewer sampling patterns than the total number of parameters. Thus, as the Examiner suggests, one or more of the parameters can have multiple sampling patterns; alternatively, there can be a single sampling pattern that defines a sampling for multiple parameters – for example, a single sampling pattern for all of the parameters together – so long as a sampling is defined for each of the parameters. The applicant submits that while this language may be broad, it is not indefinite.

The Examiner next points to the recitation in claim 1 and a number of other claims that a plurality of the parameters are “grouped according to a parameter type such that the grouped parameters are constrained to perform a common role”, and states that it is unclear what is meant by “to perform a common role”. The applicant first notes that the ordinary meaning of “role” is “a function performed by someone or something in a particular situation, process, or operation”. *See Webster's Third New International Dictionary* (1992), at page 1968. The applicant submits that in the context of the present claims, one skilled in the art would readily recognize that this language simply requires that a plurality of the parameters are grouped such that they will perform a common function in the particular experiments being designed. The specification makes this even more clear, explaining that parameters can be grouped using “type constraints” according to any of a variety of features, such as reactivity, valence state, function, and the like, that relate to their role in the set of experiments. *See Specification* at page 22, lines 25-28. Thus, in one example described in the specification starting at page 26, line 26, six starting materials A through F are grouped into three types TM, M and RE in an experiment design for a set of

experiments intended to seek magnetic compositions made up of combinations of transition metals (TM), metalloids (M) and rare earth elements (RE). As explained in the specification, after defining and grouping the six parameters according to the roles that the materials are expected to play in the target compositions – here, grouping materials A, B and C in type TM, materials D and E in type M, and material F in type RE, *id.*, at page 27, lines 3-4, the scientist defines and subsequently modifies a sampling pattern for the parameters, and then defines a number of different constraints. *Id.*, at page 27, lines 5-23. As the explanation makes clear, because parameters A, B and C are grouped as type TM, they are treated together in the subsequent experiment design process, such that a sum constraint on the total fractional composition of these materials requires that together the type TM parameters make up more than 50% of the composition in each experiment, and that the TM parameters are sampled with a step size of 10%. *Id.*, at lines 14-16; 19-21. The applicant submits that based on the ordinary meaning of the claim language itself, and on this and other passages in the specification, one skilled in the art would understand that the claims simply require that a plurality of the parameters in the set of parameters must be grouped such that they will perform a common function in the experiments being designed.

The Examiner writes that the statement that the first estimate of practicability “includes” a count of the set of experiments renders the claims indefinite. The applicant submits that this language clearly requires that the estimate includes at least a count of the number of experiments in the corresponding set of experiments, as is described, for example, at page 19, lines 12-13 of the specification, which notes that the design program can provide an estimate of the number of experiments that will be required to satisfy the experimental design. While the estimate can also include additional information – such as whether the calculation of the combinatorial expansion exceeds a predetermined computational threshold relating the time required to compute a combinatorial expansion with the time taken to actually execute experiments – this does not render the claim indefinite.

The Examiner also notes that the claims do not recite any particular information that must be included in the second estimate of practicability. Claims 1 and 39 have been amended to

recite that the second estimate, like the first estimate, includes a count of the corresponding set of experiments.

Next, the Examiner points to the language “the sets of values” in a number of the claims. Claims 1, 39, and 90 have been amended to replace this language with “sampling patterns”, referring to the sampling patterns defined in the first limitation of the claim.

The Examiner also states that claims 36 and 66 do not make use of the property values recited in that claim. The applicant submits that these claims as amended clearly recite that the values in question are received as part of the input defining the set experimental parameters, which is later used in the generation of estimates of practicability as well as the final experiment design.

The Examiner states that claim 2 is indefinite because it is unclear whether the computer program is required to have instructions operable to cause the implementation of the experiment design. Claim 2 and analogous claims 95, 97 and 99 have all been cancelled.

The Examiner next points to the phrase “parameters of a specified type”, which appears in claims 11, 12, 45 and 46. These claims specify that the constraints include type constraints (claims 11 and 45) or sum constraints (claims 12 and 46), which limit the total number of parameters of a specified type or the sum of a contribution of parameters of a specified type, respectively. The applicant submits that the “metes and bounds” of “specified type” in any given instance are defined by a user who defines the type – for example, by defining a type constraint as recited in claims 11 and 45. The specification explains that “[t]ype constraints group parameters into types (*e.g.*, such that two parameters of the same type are not both present in individual experiments returned by design program 130).” *See* Specification at page 16, lines 28-30. As the specification further explains, “[t]ype constraints permit the user to ‘group’ similar parameters by a variety of common features relating to the parameter’s role in the set of experiments (*e.g.*, by grouping chemicals by reactivity, valence state, function or the like). The inclusion of type constraints can streamline the process of calculating the combinatorial expansion, in essence requiring only a single calculation for all members of a given group or type, with the resulting set of experiments being permuted for each group member.” *Id.*, at page 22, lines 25-31. Similarly, the specification explains that sum constraints can be defined to

specify a range for the sum of all parameters of a particular type. *Id.*, at page 23, lines 1-5.

Thus, to take the Examiner's hypothetical example, whether parameters representing copper and fluorine are of the same specified type in any given instance, and for what reason, depends on how the type is (or types are) specified by the user. The applicant submits that this does not render the claims indefinite.

The Examiner next points to language in claims 13, 47 and 98 describing balance constraints, stating that the claims do not recite how or under what circumstances such a constraint might limit the contribution of a parameter based on contributions of other parameters to the experiment design. The applicant submits that the language in question simply provides that the balance constraint limits the contribution of one or more parameters to experiments in the set of experiments based in some way on the contribution of some other parameter or parameters to those experiments. The specification explains that "[b]alance constraints can be invoked to constrain one element of a combination (*e.g.*, a member of one group in a multi-group combination such as may be defined using a set of type constraints . . .)." *See* Specification, at page 18, lines 12-14. The specification provides a specific example, in which the amount of a material C to a desired composition ABC is constrained based on the combined contribution of materials A and B, such that the amount of $C = 100\% - A - B$. *Id.*, at lines 15-27. The applicant submits that no more particularity is required.

The Examiner next points to the use of "including" in the phrase "selected from the group including" claim 23. Claim 23 has been amended to delete "including", such that the claim recites that the constraints include one or more constraints selected from the listed types of constraints.

Finally, the Examiner points to language in claims 38 and 68 reciting that the material properties associated with a component material (as recited, for example, in claim 36) can include types describing classes of chemicals to be used in generating the experiment design. The applicant submits that just what constitutes a "class" of chemicals can depend on the particular chemistry involved, but that the scope of the term would be apparent in any given case to one skilled in the art. For example, in the magnetic compositions example discussed at pages 26-27 of the specification, classes of chemicals might include transition metals, metalloids and

rare earths. In other cases, classes of chemicals might similarly include, for example, alkaline earth metals, halogens, acids, bases, alcohols, esters, or other categories or groupings based on any number of chemical properties or characteristics that would be familiar to chemists in different disciplines.

The applicant submits that the claims are not indefinite and asks that the rejection under section 112, paragraph 2 be withdrawn.

4. Information Disclosure Statements

The applicant notes that Information Disclosure Statements were submitted on May 15 and May 28, 2003, and requests that the references cited therein be considered and that initialed copies of the corresponding lists on Form 1449 be returned to the applicant's undersigned representative.

Applicant : Marco Falcioni, et al.
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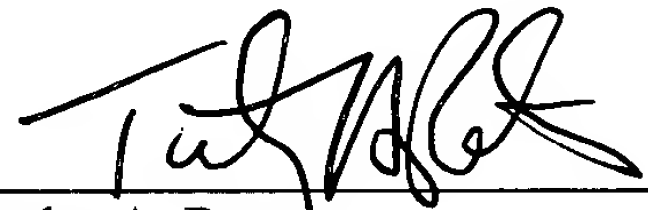
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5. Conclusion

Enclosed is a check for excess claim fees and a \$210.00 check for the Petition for Extension of Time fee. Please apply any other charges or credits to deposit account 06-1050.

Respectfully submitted,

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